MICROSCOPIC SIMULATIONS OF SHOCK PROPAGATION IN CONDENSED MEDIA: COMPARISON BETWEEN REAL TIME AND FREQUENCY DOMAINS

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MICROSCOPIC SIMULATIONS OF SHOCK PROPAGATION IN CONDENSED MEDIA:

COMPARISON BETWEEN REAL TIME AND FREQUENCY DOMAINS*

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Computer molecular dynamics (CMD) is now recognized as a very powerful technique for examining the microscopic details of a wide variety of chemical and physical phenomena, including the shock-induced fast decomposition processes that characterize the shock-initiation of energetic materials. The purpose of the present paper is to describe some results obtained by new methods of post processing of CMD data. First we present a pictorial history of a canonical system which is bonded with identical potentials and has identical atomic masses. We then present Fourier transforms of the energy components of different units judiciously chosen to show the "frequency fingerprint" of the shock impact and passage through specific units of the system, including, e.g., the behavior of spalled fragments.

To complement these studies, we also display the behavior of our canonical system when defects (point or line) are present. In these studies we monitor the motion of diatoms above and below a line defect consisting of heavy masses. The Fourier transform techniques provide optimum compromise histories which present neither too much nor too little detail.

1. INTRODUCTION

Of the three/four states of matter: solid, liquid and gas/plasma, the last differs far more radically from the first two than the first two do from each other. The primary difference, from which all others largely spring, is that of density or volume/particle. While this is essentially unchanged at the solid-liquid transition, at the liquid (or solid)-gas transition the volume/particle ratio increases by many orders of magnitude (at least by 10^5 and often by far more). Consequently, the zero order theoretical approximation is that of an assembly of largely non-interacting free particles (the "ideal gas"). This has the consequence that workers dealing with shock phenomena in gases recognize, either explicitly or implicitly, that there are fundamental limitations on the continuum hydro-codes used to model hydrodynamic phenomena, and that shock fronts are beyond those limits. As a consequence of this realization, the shock is regarded as a discontinuity about which hydro-codes can say essentially nothing and is simply modelled by imposing the Hugoniot jump conditions across the shock front.

The recognition of this limitation stems from a proper understanding of gaseous behavior which acknowledges that thermodynamic concepts, such as pressure and temperature, can only be defined for regions large compared with the mean free path of molecules in the gaseous phase. Since shock fronts arise from non-linearities in the basic (Navier-Stokes) equations, they will automatically steepen until their width is at the mean free path limit. Thus the front is recognized as a special region whose full understanding can only be achieved by a detailed examination of the microscopic behavior of the molecules in the shock region. Specifically, it comes as no surprise that collisions between them can lead to bond rupture, even though the temperatures behind and in front of the shock are well below that required for thermal dissociation.

The study of shocks in condensed matter has suffered from the lack of any such clear-cut criterion. Thus, hydrocode studies of shock propagation in solids are carried through with the inclusion of a viscous (lossy) damping in the equations and typically give shock widths of millimeters and rise times of microseconds, both of which appear to agree with experiment. However, 0.5 mm/μsec = 5.0 Å/picosecond. Thus, if we have a front which is composed of a sequence of "steps" of width $\sim$ interatomic spacing, it will appear to show a microsecond rise time if it is examined by probes which are of millimeter dimensions; however, what these observations are actually reflecting are the natural time and frequency scales of interatomic motion.

Once this is realized it is apparent that the hydro-codes are being forced beyond the same natural limit as that for gaseous media; namely, the mean interatomic spacing which, in condensed materials, fills the same role as the mean free path in gases. The proper way to resolve this difficulty is to examine the propagating shock front at the microscopic (atomic) level; experimentally, this is beyond the limits of spatial and temporal resolution currently available simultaneously, although recent work has demonstrated that when both "windows" (limits) are reduced, the shock width shrinks in the manner we would predict. However, it is both easier and much cheaper to do a computer experiment using the techniques of computer molecular dynamics (CMD). These involve setting up in the computer the Newton's law equations of motion for an assembly of atoms bound in regular or irregular arrays and numerically integrating them to determine the system's temporal history, following initial impact loading.

Over the past ten years, we have carried out many such studies,[1] but most recently[2,3] we have been concerned with developing post-processing techniques that will enable us to present in a compact and manageable form the temporal histories of each simulation, without resorting to such broad averaging that the detailed behavior of the shock is lost or obscured. It is in the nature of the these simulations that they contain all possible information, and one can scan this by generating a movie of each history--however, this provides qualitative rather than quantitative insight.

In this paper we wish to present early results of applying two post-processing techniques both to one of our original canonical studies and to a related simulation designed to show the effects of lattice irregularities or defects.

2. NATURE OF THE SIMULATIONS

The techniques of CMD are now well documented by both others and ourselves.[1,4] The only novel features are the use of "neighborhood look-up"

procedures to keep track of the interatomic bonding, and the use of various post processing options such as Fourier transforms of the energy components of different units or regions of our assembly.

2a. STUDIES OF THE IDEAL SYSTEM

This consists of a regular two-dimensional array of atoms all identical and identically bonded to their first and second neighbors.* This array is shocked by bringing in with uniform velocity from the left a "plate" made up of an identical lattice. We then examine the temporal evolution of the system. In Fig. 1, we show selected stills from a movie history of the system which are of interest in their own right, since, in our original simulation, we had no provision for "look up" (a procedure which periodically updates the bonds retained); thus the configurations at later times, when radical particle rearrangements have taken place, were unrealistic.

We next proceeded first to tag the single atom indicated in Fig. 1 and then to tag the whole spall as a single unit. In Fig. 2, we show the energy flux into and out of the motion of the single tagged atom as the shock passes it, and the flux of energy into the spalled end as the spall developes. (A pointed end was chosen as displaying the most interesting behavior.)

These histories of energy flux permit genqral statements, but they also show that they are neither the clearest nor most compact presentations. Fairly clearly one has a number of sinusoidal, or near-sinusoidal, oscillations superposed. Given this situation in the temporal domain, the natural method of data reduction is that appropriate to signal processing: the Fast Fourier Transform (FFT). This provides a "fingerprint" identification of the various types of characteristic frequencies in any given atomic/molecular process.

These transforms are shown in Figs. 3 and 4 for the single atom and the spall. In order to retain sufficient temporal discrimination to display separately clearly distinct parts of the history (e.g., before and after spall), the temporal range was split into segments, and each was separately transformed. The most interesting feature is the rapid build up of higher frequency components in the spall motion as time proceeds.

2b. STUDIES ON IMPERFECT SYSTEMS

In view of the importance of the interactions of shocks with lattice irregularities or surfaces, processes which seem to provide the most efficient means of conversion of shock-energy into single atom/radical energy, we decided to examine the behavior of our canonical system when we introduced a line defect. We, therefore, set up the situation shown in Fig. 5 in which we have a line defect (for simplicity represented by heavy substitutional atoms of mass 100, a zero order approximation to a dislocation or twin boundary), and monitored two diatomic units situated such that one (the lower) is unshielded by the line defect and the other shielded. The shock was launched by the standard plate impact method. For brevity, we only show the transform (windowed as before) for both tagged diatoms in Fig. 6.

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*We have the capability to study three-dimensional systems. In initial, survey types of calculations it is much more economical to restrict ourselves to two-dimensional systems. The addition of the third dimension introduces quantitative rather than qualitative changes.

It should be noted that the "shelter" is not particularly efficient: the reason for this is that the line of heavy atoms so distorts the shock front that considerable energy is projected diagonally upwards into the "sheltered" region. It is, however, apparent that the higher frequency components are suppressed in the sheltered region. Thus, it is evident that the shielding is most efficient for the higher frequency components of the motion.

3. CONCLUSIONS

The present rather preliminary studies clearly demonstrate the potential usefulness of the FFTs as a means of data reduction. The actual histories studied here have no very dramatic features, but they demonstrate clearly that high frequency molecular motions are readily excited by shock loading; however, such high frequency motions are more inhibited in their motion by heavy defects, or, probably, "soft" bonds.

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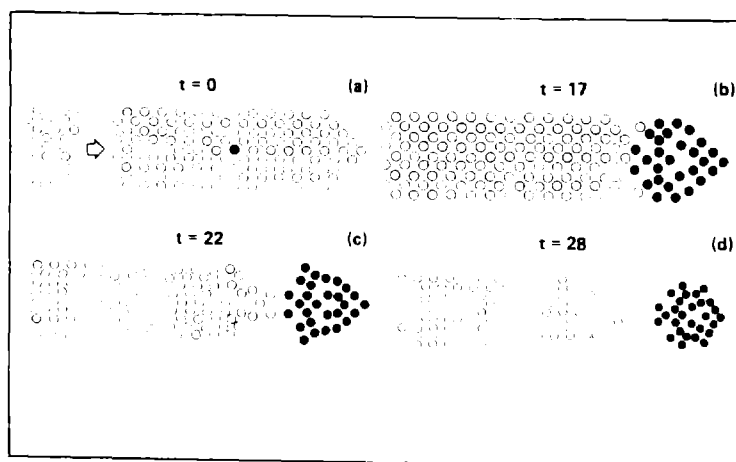
Figure 1. Configurations for a shocked monoatomic lattice (time in units of 10^{-14} s): a) t = 0 shows tagged atom; b) t = 17; c) t = 22; d) t = 28.
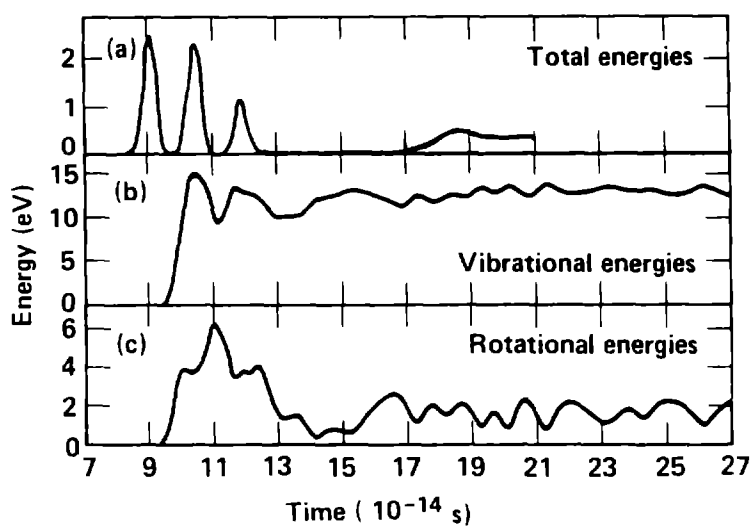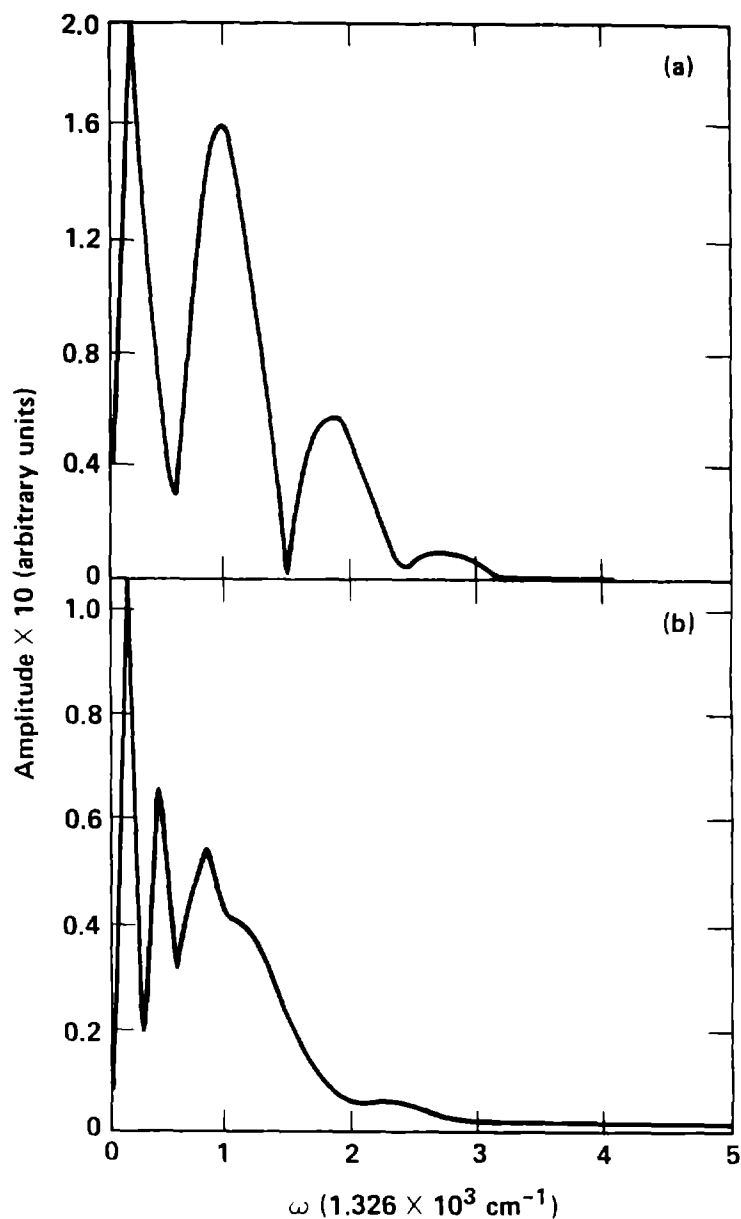
Figure 2. Histories of the vibrational energy: a) For the single tagged atom; b) For the spalled fragment; c) History of the rotational energy of the spalled unit.

Figure 3. Fast Fourier transforms (FFTs) for the vibrational energy of the atom tagged during the Fig. 2 run (time in units of 10^{-14} s): a) FFT, t = 0-10; b) FFT, t = 10-20.
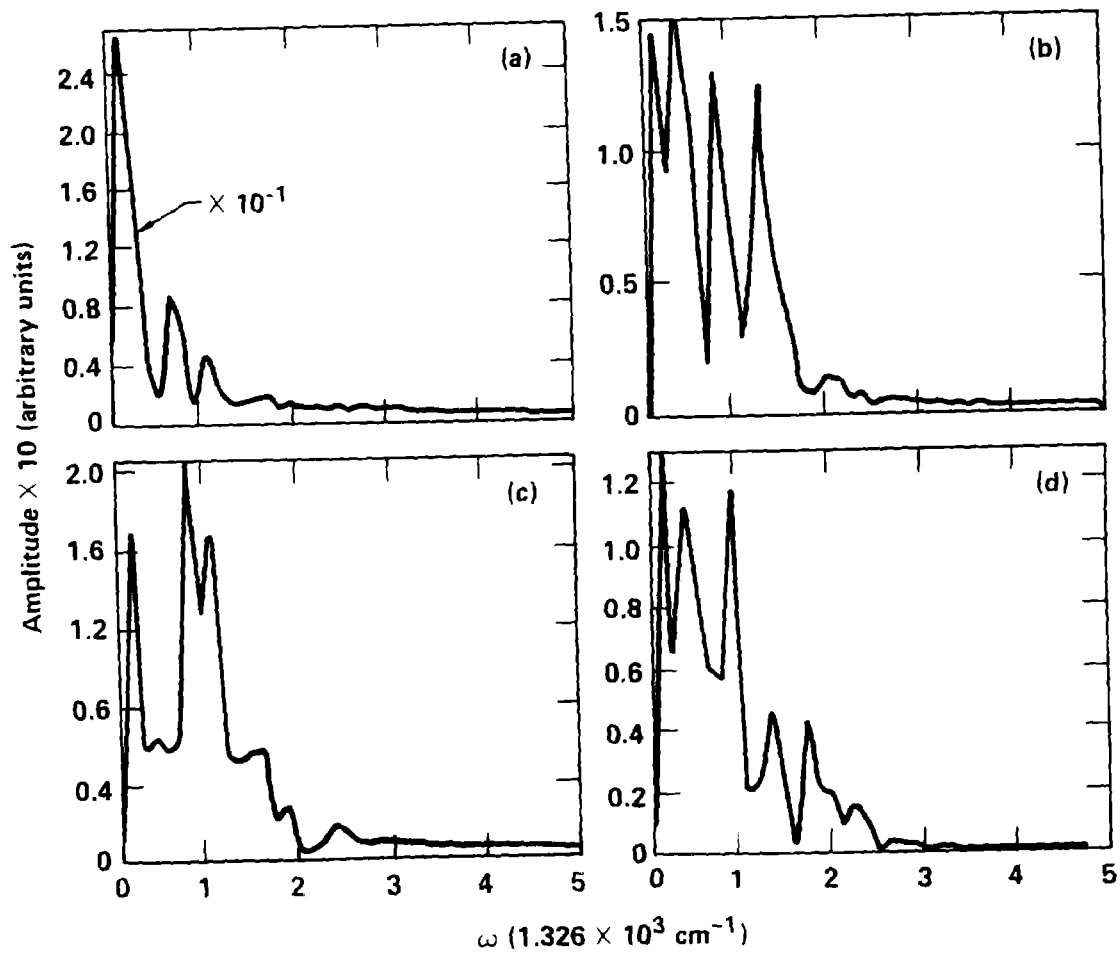
Figure 4. FFTs of the vibrational energy of the spalled fragment (time in units of 10^{-14} s): a) t = 7-17; b) t = 17-27; c) t = 28-38; d) t = 38-48. Note the build up of higher frequency components after spall.
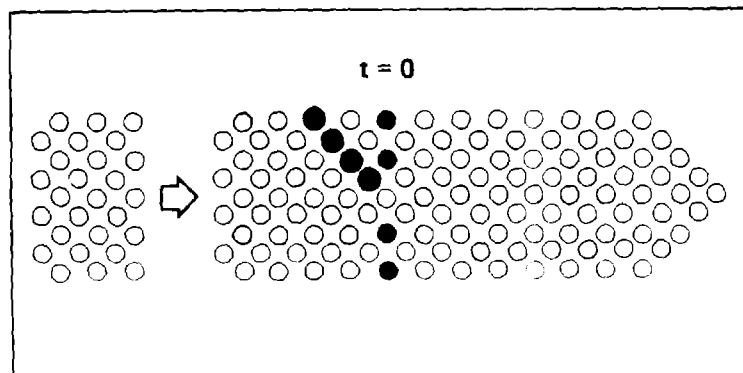

Figure 5. Initial configuration for the shock impact on an imperfect system showing the line defect (mass 100 atoms) and the two diatoms whose vibrational energy is tagged.
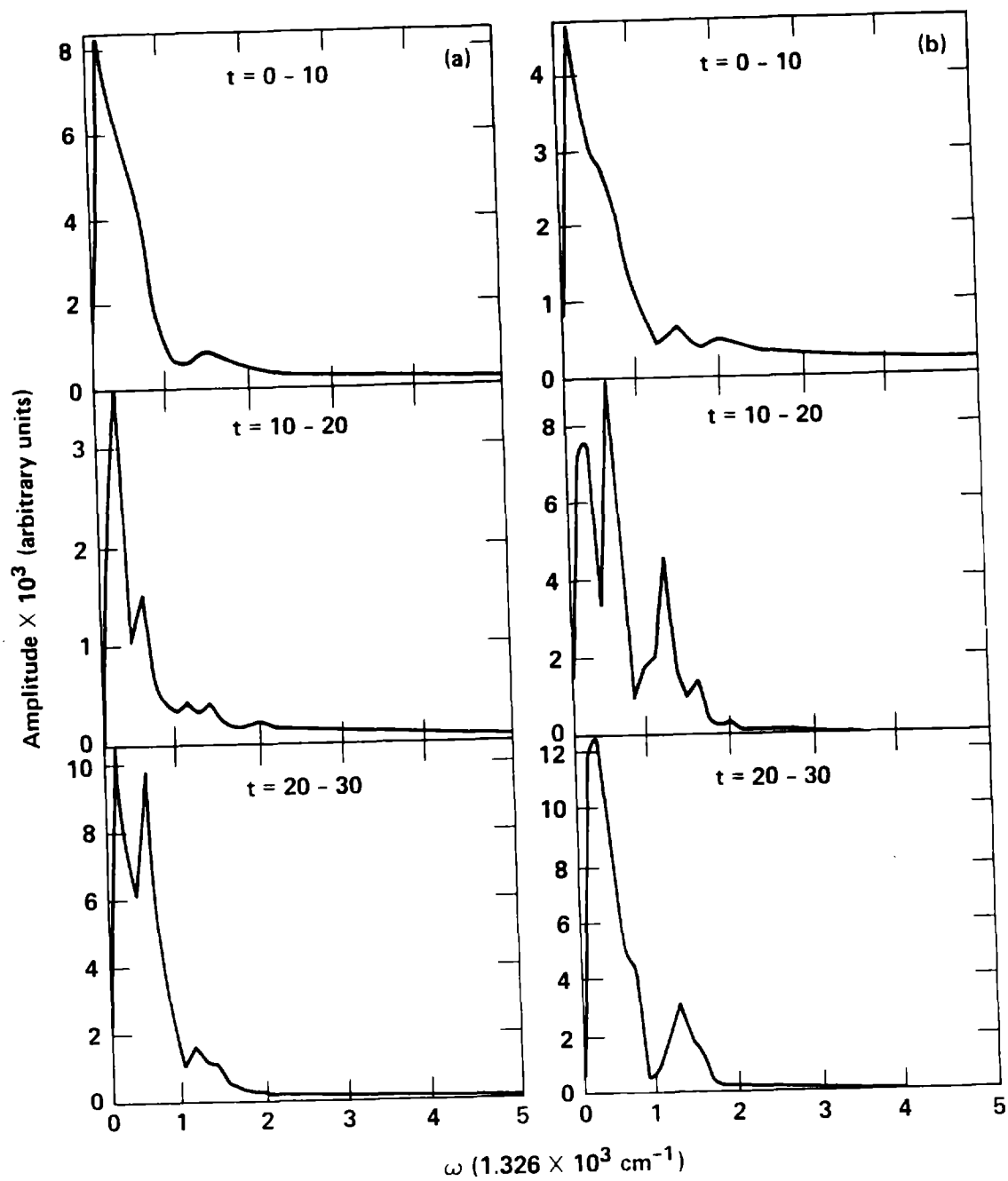
Figure 6. FFTs of the diatom vibrational energies: a) "Sheltered" (upper) diatom; b) "Exposed" (lower) diatom.